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Analytical Solutions for Convection-Diffusion-Dispersion-Reaction-Equations with Different Retardation-Factors and Applications in 2d and 3d[1]

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Abstract

Our motivation to this paper came from a model simulating a waste-disposal embedded in an overlying rock. The main problem for our model are the large scales that occurred due the coupled reaction terms of our underlying system of convection-diffusion-dispersion-reaction-equations. The developed methods allowed a computation over a large simulation period of more than 10000 years. Therefore we construct discretization methods of higher order, which allow large-time-steps without loss of accuracy. Based on operator-splitting methods we decouple the complex equations in simpler equations and use adequate methods to solve each equation separately. For the explicit parts that are the convection-reaction-equations we use finite-volume methods based on flux-methods with embedded analytical solutions. Whereas for the implicit parts that are the diffusion-dispersion-equations we use finite-volume methods with central discretizations. We analyze the splitting-error and the discretization error for our methods. The main part of the paper consists of the applications of our methods done with our underlying program-tool R^3T. We introduced the main concepts of the program-tool that is based on the software-toolbox UG. The test-examples and benchmark problems for verifying our discretization- and solver-methods with respect to the physical behavior are presented. The benchmark-problems are the test for different material-parameters and confirm the valuation of the methods. Based on the verification of our

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test-problem we present the realistic model-problem of a waste-disposal in 2d with large decay-chains reacted and transported in a porous media with an underlying flowing groundwater. For the prediction of possible waste-disposals a computation with different located waste-locations is discussed. The parallel resources for the computations are presented in the case of the forced simulation-times.

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1 Introduction

We are motivated for our studies to understand the transport and reaction processes from the realistic background of a waste-disposal for radioactive contaminants transported with flowing groundwater through an overlying rock. For this complex model the equations are derived and we describe the solver and discretization methods for the different convection and diffusion dominant cases. For a full description we also present the solvers for the nonlinear equations. The main idea for such complex equations is the idea to split the complex equation in simpler equations and to solve these equations with higher accuracy. The operator-splitting methods are used to solve such complex coupled equations. We split the multi-physical and multidimensional equation in simple-physical and one-dimensional equations. The methods are presented for first or higher order methods with respect to the forced accuracy. Based on this splitting method the simpler equations are discretized with adapted methods to obtain a higher order accuracy for the partial parts. The discretization methods are adapted with respect to the equations. We use explicit time-discretization and finite volume method for the convection-equation. An explicit time-discretization with a modified finite volume method is used for a linear convection-reaction equation. The linear and nonlinear reaction equations are analytically solved, because of their solvability as ordinary differential equations. For the diffusion-dispersion equation we use implicit time-discretization and standard finite volume methods. The underlying linear system of equations is solved iteratively with a multi-grid solver. Our main advantage in this context is the coupling of the different equation-types to obtain higher order discretization methods.

For the application of our methods we present the underlying software package R^3T. The concept is the flexibility and the decomposability of different

discreti-zation- and solver-methods. We introduce the concept of this software package and the application for test-examples with various parameters.

We applied our methods for applications in waste disposals. A new benchmark-example for a waste-disposal is presented with realistic parameters. Further we introduce a new example for a 2d waste-disposal with 2 sources and different layers. The calculations are presented with figures and convergence results.

The paper is outlined as follows. We introduce our mathematical model of contaminant transport in flowing groundwater in section 2. The various operator-splitting methods for the complex equation to simpler equations are described in section 3. In section 4 we introduce the discretization methods for our different equations and explain embedding methods for special convection-reaction equations. The analytical solutions for reaction and linear convection-reaction equations are discussed in the section 5. We introduce the numerical solvers and concentrate on the multi-grid solver in section 6. The software-package is presented in section 7. Our numerical results with benchmark-problems and realistic waste disposals are described in section 8. Finally we discuss our future works in this area.

2 Mathematical Model

The motivation for the study presented below is coming from a computational simulation of radionuclide contaminants transport in flowing groundwater [6], [9].

The mathematical equations are given by

$$\partial_t\, R_\alpha(c_\alpha) + \nabla \cdot (\mathbf{v} c_\alpha - D\nabla c_\alpha) + \lambda_{\alpha\beta}\, R_\alpha(c_\alpha) = \sum_{\gamma\in\gamma(\alpha)} \lambda_{\gamma\alpha}\, R_\gamma(c_\gamma)\ , \tag{1}$$

$$R_\alpha(c_\alpha) = (\phi + (1-\phi)\rho K(c_\alpha))\ c_\alpha\ , \tag{2}$$

$$\text{with}\ \ \alpha = 1, \ldots, m\ . \tag{3}$$

The unknowns $c_\alpha = c_\alpha(x,t)$ are considered in $\Omega \times (0,T) \subset I\!R^d \times I\!R$, the space-dimension is given by d . ϕ is the porosity, ρ is the density. The retardation $R_\alpha(c_\alpha)$ is given as a linear or nonlinear function. For the linear retardation we have the Henry-Isotherm with $K(c_\alpha) = K_d^\alpha$, where K_d^α is the element-specific K_d-parameter. We simplify the model and assume for each element one isotope, confer our complex model [14]. For the nonlinear retardation-factor we have the Freundlich-Isotherm with $K(c_\alpha) = K_{nl}(c_\alpha)^{p-1}$, where K_{nl} is the specific sorption-constant and p is the exponent of the isotherm. Another nonlinear retardation-factor is the Langmuir-Isotherm with $K(c_\alpha) = \frac{\kappa\, b}{1+b\, c_\alpha}$, where b is the specific sorption-constant and κ is the specific sorption-capacity. The other parameters are $\lambda_{\alpha\beta}$ the decaying rates from α to β, where $\gamma(\alpha)$ are the predecessor-elements of element α. D is the Scheidegger diffusion-dispersion tensor and $\mathbf{v}$ is the velocity.

The main aim of this paper is to present new methods, which are based on exact solutions for simpler one-dimensional equations. For this purpose we derive analytical solutions for the simpler one-dimensional convection-reaction equation and also for the nonlinear reaction-equations. The analytical solutions are used for the explicit time-discretization and spatial-discretization with finite volume methods for d-dimensions.

A higher order-method for the linear convection-reaction-equation is derived with the idea to embed the analytical solution of the mass to our finite volume discretization. The mass-transport coupled the convection-reaction-equation together. For the nonlinear retardation our methods are based on the operator-splitting methods of higher order. We could couple analytical solutions for the nonlinear reaction-equation with the convection-diffusion equation together. For these coupling methods we also get higher order methods, which allow larger coarser-grids with larger time steps. We could therefore fulfill the forced long time-period calculations, e.g. scenarios about 10000 years are calculate-able in one day.

The higher order finite volume method is based on TVD methods and is constructed according to the discrete minimum and maximum principle that is used by the new methods to reach second order for all components.

For the derivation of our new methods based on the embedding of one-dimensional analytical solution for convection-reaction-equations we use the d-dimensional convection-reaction equations with equilibrium sorption.

So the equation for this linear case is given by:

$$R_i \partial_t c_i + \nabla \cdot (\mathbf{v} c_i) = -\lambda_i R_i c_i + \lambda_{i-1} R_{i-1} c_{i-1} \ , \ i = 1, \ldots, m \ , \tag{4}$$

$$c_i = (c_{1,i}, \ldots, c_{d,i})^T \in I\!R^d \ , \tag{5}$$

where $R_i \geq 0$ is a constant retardation-factor. The trivial inflow and outflow boundary conditions are given by $c = 0$ and the initial conditions $c_i(x, 0) = c_{i,0}(x)$ are given as rectangular-, trapezoidal- and also polynomial-impulses and make it possible to derive the analytical solutions. Based on the one-dimensional convection-reaction equation with equilibrium sorption and initial impulses, we derive the new discretization methods, confer [14].

The following section describes the operator-splitting methods as a basic method for our new discretization methods.

3 Operator-Splitting Methods

The operator-splitting methods are used to solve complex models in the complex geophysical and environmental problems, confer [25], [27] and [30]. In this article we introduce the idea to derive simpler equations with respect to construct higher order discretization methods for the complex equations. For

this aim we use the operator-splitting method and decouple the equation as follows described.

3.1 Splitting methods of first order (sequential splitting)

The following splitting methods of first order are described. We consider the following ordinary linear differential equations:

$$\partial_t c(t) = A\ c(t)\ +\ B\ c(t)\ , \tag{6}$$

where the initial-conditions are $c^n = c(t^n)$. The operators A and B correspond to the spatially discretized equations, e.g. the convection-equation and the diffusion-equation are discretized with finite volume methods.

The operator-splitting method is introduced as a method which solves the two equation-parts sequentially and couples the equations with the initial conditions. We get two sub-equations :

$$\begin{aligned} \frac{\partial c^*(t)}{\partial t} &= Ac^*(t)\ , \quad \text{with } c^*(t^n) = c^n\ , \\ \frac{\partial c^{**}(t)}{\partial t} &= Bc^{**}(t)\ , \quad \text{with } c^{**}(t^n) = c^*(t^{n+1})\ , \end{aligned} \tag{7}$$

where the time-step is $\tau^n = t^{n+1} - t^n$. The solution of the equations is $c^{n+1} = c^{**}(t^{n+1})$.

The error of this splitting method is derived as, confer [14],

$$\begin{aligned} \rho_n &= \frac{1}{\tau}(\exp(\tau^n(A+B)) - \exp(\tau^n b)\exp(\tau^n A))\ c(t^n) \\ &= \frac{1}{2}\tau^n[A,B]\ c(t^n) + O(\tau^2)\ . \end{aligned} \tag{8}$$

whereby $[A,B] := AB - BA$ is the commutator of A and B. We get an error $O(\tau^n)$ if the operators A and B do not commute, otherwise the method is exact.

3.2 Higher order Splitting methods

We could improve our method by the so called Strang-Splitting method and also iterative methods, which are of higher order, confer [25] and [22].

The Strang-Splitting method is applied as

$$\frac{\partial c^*(t)}{\partial t} = Ac^*(t)\ ,\ \text{with } t^n \le t \le t^{n+1/2} \text{ and } c^*(t^n) = c^n\ , \tag{9}$$

$$\frac{\partial c^{**}(t)}{\partial t} = Bc^{**}(t) \ , \text{ with } t^n \leq t \leq t^{n+1} \text{ and } c^{**}(t^n) = c^*(t^{n+1/2}) \ ,$$
$$\frac{\partial c^{***}(t)}{\partial t} = Ac^{***}(t) \ , \text{ with } t^{n+1/2} \leq t \leq t^{n+1} \text{ and } c^{***}(t^{n+1/2}) = c^{**}(t^{n+1}) \ ,$$

where the result of the method is $c^{n+1} = c^{***}(t^{n+1})$.

The splitting error of this method is given as, confer [20],

$$\rho_n = \frac{1}{24}(\tau^n)^2([B,[B,A]] - 2[A,[A,B]])\ c(t^n) + O((\tau^n)4) \ , \qquad (10)$$

where we get the second order if the operators do not commute and an exact result if they commute. We could improve the order by using more intermediate steps.

The Iterative-Splitting method is applied as

$$\partial_t c^i = Ac^i + Bc^{i-1} \quad \text{with} \quad c^i(t^n) = c^{i-1}(t^{n+1}) \ ,$$
$$\partial_t c^{i+1} = Ac^i + Bc^{i+1} \quad \text{with} \quad c^{i+1}(t^n) = c^i(t^{n+1}) \ ,$$

where i is the iteration-index and the initial-conditions are $c^0(t^n) = 0$ and $c^{-1}(t^{n+1}) = 0$. We define the error $e(t^{n+1}) := c^{i+1}(t^{n+1}) - c^i(t^{n+1})$ as an error-boundary for the truncation-error. We get a higher-order method as described in [22].

We apply the first order splitting for the convection-reaction- and the diffusion-dispersion-term, because of the dominant space-error. In further applications we use a higher order splitting-method to get a second-order for the time-error.

In the next section we present the different discretization methods for the equations.

4 Discretization

We use finite volume methods for the space-discretization and for the time-discretization we use explicit or implicit Euler methods. In the next section we introduce the notation for the space-discretization. Furthermore we describe the discretization-methods for the further different equation-terms.

4.1 Notation for the Discretization

The time steps for the calculation in the time intervals are $(t^n, t^{n+1}) \subset (0, T)$, for $n = 0, 1, \ldots$. The cells for the computations are given as $\Omega_j \subset \Omega$ with $j = 1, \ldots, I$. The unknown I is the number of the nodes.

The finite volume methods use a primary and dual mesh to construct the method. We have to construct the dual mesh for the triangulation $\mathcal{T}$ [11] of the domain Ω. The primary mesh is given for the finite elements in the domain Ω by $T^e, e = 1, \ldots, E$. The polygonal computational cells Ω_j are related with the vertices x_j of the triangulation.

For the relation between the neighbor cells and the volumes of each cell we introduce the following notation. Let $V_j = |\Omega_j|$ and the set Λ_j denotes the neighbor-point x_k to the point x_j. The boundary of the cells j and k is Γ_{jk}.

The flux over the boundary $?\Gamma_{jk}$ is defined as

$$v_{jk} = \int_{\Gamma_{jk}} \mathbf{n} \cdot \mathbf{v} \, ds \; . \tag{11}$$

The inflow-flux is given as $v_{jk} < 0$, the outflow-flux is $v_{jk} > 0$. We have the antisymmetry of the fluxes and denote them as $v_{jk} = -v_{kj}$. The total outflow-flux is given by

$$\nu_j = \sum_{k \in out(j)} v_{jk}. \tag{12}$$

The discretization of the finite volumes allow us to derive an algebraic system of equations and express our unknowns as $c_j^n \approx c(x_j, t^n)$. The initial values are given as c_j^0. The expression of the interpolation schemes could be given naturally in two ways. The first expression is given with the primary mesh of the finite elements:

$$c^n = \sum_{j=1}^{I} c_j^n \phi_j(x), \tag{13}$$

where ϕ_j are the standard globally finite element basis functions [11]. The second expression is possible with the finite volumes and is given as,

$$\hat{c}^n = \sum_{j=1}^{I} c_j^n \varphi_j(x) \tag{14}$$

where φ_j are piecewise constant discontinuous functions defined by $\varphi_j(x) = 1$ for $x \in \Omega_j$ and $\varphi_j(x) = 0$ otherwise.

4.2 Discretization of the convection-equation with first order test-functions

We use the piecewise constant test-functions for the discretization of the convection equation

$$\partial_t R \, c - \mathbf{v} \cdot \nabla c = 0 \; , \tag{15}$$

with the simple boundary condition $c = 0$ for the inflow and outflow boundary and the initial values $c(x_j, 0) = c_j^0(x)$. We derive the following equation with the upwind discretization done in [11]:

$$V_j \; R \; c_j^{n+1} \;\; = \;\; c_j^n (R \; V_j - \tau^n \nu_j) + \tau^n \sum_{k \in in(j)} R \; c_k^n \; v_{kj} \; . \tag{16}$$

Because of the explicit time-discretization we have to fulfill the discrete minimum-maximum property [11]. We get a restriction for the time steps as follows

$$\tau_j = \frac{R \; V_j}{\nu_j} \; , \;\; \tau^n \leq \min_{j=1,\ldots,I} \tau_j \tag{17}$$

To derive a higher order method for our underlying discretization method, in the next subsection we explain a reconstruction of the constant test-functions with linear polynomials. The reconstruction is based on the Godunovs method and the limiter on the local min-max property.

4.3 Discretization of the convection-equation with a reconstruction to higher order methods

The reconstruction is done in the paper [11] and is here briefly explained for the next steps.

The linear polynomials are reconstructed over the element-wise gradient, confer [23], and are given as

$$u^n(x_j) = c_j^n \; , \tag{18}$$

$$\nabla u^n|_{V_j} = \frac{1}{V_j} \sum_{e=1}^{E} \int_{T^e \cap \Omega_j} \nabla c^n dx \; , \tag{19}$$
$$\text{with} \quad j = 1, \ldots, I \; .$$

The piecewise linear functions are given by

$$u_{jk}^n = c_j^n + \psi_j \nabla u^n|_{V_j} (x_{jk} - x_j) \; , \tag{20}$$
$$\text{with} \quad j = 1, \ldots, I \; ,$$

where $\psi_j \in (0, 1)$ are the limited parameters, which have to fulfill the discrete minimum maximum property.

The piecewise linear functions are given by

$$u_{jk}^n = c_j^n + \psi_j \nabla u^n|_{V_j} (x_{jk} - x_j) \; , \quad j = 1, \ldots, I \; ,$$

where $\psi_j \in (0, 1)$ is the limiter, which has to fulfill the discrete minimum-maximum property, as described in [11].

We also use the limitation of the flux to get no overshooting, when transporting the mass and receive the maximal time-step.

The restrictions for the concentration are given as

$$\tilde{u}_{jk}^n = u_{jk}^n + \frac{\tau_j}{\tau^n}(c_j^n - u_{jk}^n) \ . \tag{21}$$

Using all the previous schemes the discretization for the second order is written in the form

$$RV_j c_j^{n+1} = RV_j c_j^n - \tau^n \sum_{k \in out(j)} \tilde{u}_{jk}^n v_{jk} + \tau^n \sum_{l \in in(j)} \tilde{u}_{lj}^n v_{lj} \ . \tag{22}$$

We improve the discretization of the convection-equation by embedding the reaction-equation and derive a higher order method for the convection-reaction equation. This discretization method is constructed without using the operator-splitting method and therefore we could skip the former splitting-error.

4.4 Discretization of the convection-reaction-equation with embedded one dimensional analytical solutions

We apply the one-dimensional Godunovs method for the discretization, confer [23], and enlarge it with the solution of convection-reaction-equations. We add the solutions for the reaction-equation to our convection-equation. We reduce the equation to one-dimensional problem, solve the equation exactly and transform the one-dimensional mass to the multi-dimensional equation.

The discretization of the equation is denoted as

$$\partial_t \ c_l + \nabla \cdot \mathbf{v}_l \ c_l = -\lambda_l \ c_l + \lambda_{l-1} \ c_{l-1}, \quad \text{with } l = 1, \ldots, m.$$

The velocity vector $\mathbf{v}$ is divided by R_l. The initial conditions are given as $c_l^0 = c_l(x, 0)$ for $l = 1$ and $c_l^0 = 0$ for $l = 2, \ldots, m$. The boundary conditions are trivial and given as $c_l = 0$ for $l = 1, \ldots, m$.

The maximal time-steps over all cells are first calculated. The time step for cell j and concentration i with the use of the total outflow fluxes is denoted as

$$\tau_{i,j} = \frac{V_j \ R_i}{\nu_j} \ , \quad \nu_j = \sum_{k \in out(j)} v_{jk} \ .$$

We get the restricted time step for the local time steps of each cells and their components. They are calculated with the minimum over each time-step and are given as

$$\tau^n \leq \min_{\substack{i=1,\ldots,m \\ j=1,\ldots,I}} \tau_{i,j} \ .$$

The velocity of each discrete equation is given by

$$v_{i,j} = \frac{1}{\tau_{i,j}} \ .$$

We could calculate the analytical solution of the mass, because we derive the analytical solution of the concentrations, confer section 5 by using equation (49) and (51). We denote the mass-function as

$$\begin{aligned} m^n_{i,jk,out} &= m_{i,out}(a, b, \tau^n, v_{1,j}, \ldots, v_{i,j}, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i) \ , \\ m^n_{i,j,rest} &= m^n_{i,j} \ f(\tau^n, v_{1,j}, \ldots, v_{i,j}, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i) \ , \end{aligned}$$

where $a = V_j R_i (c^n_{i,jk} - c^n_{i,jk'})$, $b = V_j R_i c^n_{i,jk'}$ and $m^n_{i,j} = V_j R_i c^n_{i,j}$ are the parameters. The linear impulse in the finite-volume cell is given by $c^n_{i,jk'}$ for the concentration on the inflow- and $c^n_{i,jk}$ for the concentration on the outflow-boundary of the cell j.

The improved discretization with the embedded analytical mass is calculated by

$$m^{n+1}_{i,j} - m^n_{i,rest} = - \sum_{k \in out(j)} \frac{v_{jk}}{\nu_j} \, m_{i,jk,out} + \sum_{l \in in(j)} \frac{v_{lj}}{\nu_l} \, m_{i,lj,out} \ ,$$

where $\frac{v_{jk}}{\nu_j}$ is the re-transformation of the total mass $m_{i,jk,out}$ in the partial mass $m_{i,jk}$. The mass in the next time-step is $m^{n+1}_{i,j} = V_j \, c^{n+1}_{i,j}$ and in the old time-step it is the rest mass for the concentration i . The proof is done in [14].

In the next section we describe the discretization for the reaction-equations, which are solutions for systems of ordinary differential equations.

4.5 Discretization of the Reaction-equation

The reaction-equation is an ordinary-differential equation and is given as follows:

$$\partial_t R_i c_i = -\lambda_i R_i c_i + \lambda_{i-1} R_{i-1} c_{i-1} \ , \tag{23}$$

where $i = 1, \ldots, m$ and the initial decay-rate is given as $\lambda_0 = 0$. The decay-factors are $\lambda_i \geq 0.0$ and the constant retardation-factors are $R_i > 0.0$. The initial-conditions are $c_1(x, t^0) = c_{01}$ and $c_i(x, t^0) = 0$ with $i = 2, \ldots, m$.

We could derive the solutions for these equations, confer [3], and get the analytical solutions

$$c_i = c_{01} \, \frac{R_1}{R_i} \, \Lambda_i \sum_{j=1}^{i} \Lambda_{j,i} \exp(-\lambda_j \, t) \ , \tag{24}$$

whereby $i = 1, \ldots, m$. The solutions are defined for all $\lambda_j \neq \lambda_k$ for $j \neq k$ and $j, k \in 1, \ldots, M$.
The factors Λ_i and $\Lambda_{j,i}$ are

$$\Lambda_i = \prod_{j=1}^{i-1} \lambda_j \ , \ \ \Lambda_{j,i} = \prod_{\substack{j=1 \\ j \neq k}}^{i} \frac{1}{\lambda_k - \lambda_j} \ . \tag{25}$$

For pairwise equal reaction-factors we have derived the solution in our work [14].

In the next subsection we introduce the discretization of the nonlinear reaction-equation.

4.6 Discretization of the Nonlinear Reaction-equation

The nonlinear reaction-equation is an ordinary-differential equation and is given as follows

$$\partial_t R_i(c_i) = -\lambda_i R_i(c_i) + \lambda_{i-1} R_{i-1}(c_{i-1}) \ , \tag{26}$$

where $i = 1, \ldots, m$ and $\lambda_0 = 0$. The decay-factors are $\lambda_i \geq 0.0$ and the nonlinear retardation-factors $R_i(c_i)$ are given in section 2. The initial-conditions are $c_1(x, t^0) = c_{01}$ and $c_i(x, t^0) = 0$ with $i = 2, \ldots, m$.

For derivation of the solution we apply a transformation to a linear reaction-equation and solve the equation analytically as presented in subsection 4.5 and then we apply a Newton-solver to derive the solution for the fix-point problem. We explain the following solution steps.

To get a linear reaction equation we apply the transformation

$$u_i = R_i(c_i) \ , \tag{27}$$

where $i = 1, \ldots, m$.

We get the equations

$$\partial_t u_i = -\lambda_i u_i + \lambda_{i-1} u_{i-1} \ , \tag{28}$$

where $i = 1, \ldots, m$ and $\lambda_0 = 0$ is. The decay-factors are $\lambda_i \geq 0.0$ and the nonlinear retardation-factors $R_i(c_i)$ are given in section 2. The initial-conditions are given as $u_1(x, t^0) = R_1(c_{01})$ and $u_i(x, t^0) = 0$ with $i = 2, \ldots, m$.

We could derive the solutions for these equations, confer [3], as

$$u_i = u_{01} \ \Lambda_i \sum_{j=1}^{i} \Lambda_{j,i} \exp(-\lambda_j \ t) \ , \tag{29}$$

where $i = 1, \ldots, m$. The solutions are defined for all $\lambda_j \neq \lambda_k$ for $j \neq k$ and $j, k \in 1, \ldots, M$.
The factors Λ_i and $\Lambda_{j,i}$ are given as

$$\Lambda_i = \prod_{j=1}^{i-1} \lambda_j \ , \quad \Lambda_{j,i} = \prod_{\substack{j=1 \\ j \neq k}}^{i} \frac{1}{\lambda_k - \lambda_j} \ . \tag{30}$$

For pairwise equal reaction-factors we have derived the solution in our work [14].

We re-transform to the original variables c_i by using a Newton-solver and solve the nonlinear algebraic equation

$$u_i - R_i(c_i) = 0 \ , \tag{31}$$

where $i = 1, \ldots, m$.
The roots c_i for the algebraic equation (31) are the results of our nonlinear reaction-equation.

In the next subsection we introduce the discretization of the diffusion-dispersion-equation.

4.7 Discretization of the Diffusion-Dispersion-equation

We discretize the diffusion-dispersion-equation, because of their stabile behavior with implicit time-discretization and finite volume method. The diffusion-dispersion equation is denoted as

$$\partial_t R \, c - \nabla \cdot (D \nabla c) = 0 \ , \tag{32}$$

where $c = c(x,t)$ with $x \in \Omega$ and $t \geq 0$. The Diffusions-Dispersions-Tensor is $D = D(x, \mathbf{v})$ given by the Scheidegger-approach, confer [24]. The velocity is given by $\mathbf{v}$ and is piecewise constant in the cells. The retardation-factor is $R > 0.0$.

The boundary-values are given as $\mathbf{n} \cdot D \ \nabla c(x,t) = 0$, whereby $x \in \Gamma$ is the boundary $\Gamma = \partial\Omega$, confer [10]. The initial conditions are denoted by $c(x,0) = c_0(x)$.

We integrate equation (32) over space and time and get

$$\int_{\Omega_j} \int_{t^n}^{t^{n+1}} \partial_t R(c) \ dt \ dx = \int_{\Omega_j} \int_{t^n}^{t^{n+1}} \nabla \cdot (D \nabla c) \ dt \ dx \ . \tag{33}$$

The integration over time is done with the backward-Euler method and we could exact integrate the left-hand side of equation (33). The right-hand side is discretized with the lumping for the diffusion-dispersion term, confer [14]

$$\int_{\Omega_j} (R(c^{n+1}) - R(c^n)) \ dx = \tau^n \int_{\Omega_j} \nabla \cdot (D \nabla c^{n+1}) \ dx \ . \tag{34}$$

The equation (34) is discretized over the space with respect of using the Greens-formula and we obtain the following equation

$$\int_{\Omega_j} (R(c^{n+1}) - R(c^n))\, dx = \tau^n \int_{\Gamma_j} D\, \mathbf{n} \cdot \nabla c^{n+1}\, d\gamma\ , \tag{35}$$

where Γ_j is the boundary of the finite volume cell Ω_j. We use the approximation in space, confer [14].

The integration of equation (35) is done for finite boundary and using of the middle-point rule yields

$$V_j R(c_j^{n+1}) - V_j R(c_j^n) = \tau^n \sum_{e \in \Lambda_j} \sum_{k \in \Lambda_j^e} |\Gamma_{jk}^e| \mathbf{n}_{jk}^e \cdot D_{jk}^e \nabla c_{jk}^{e,n+1}\ , \tag{36}$$

where $|\Gamma_{jk}^e|$ is the length of the boundary-element Γ_{jk}^e. The gradients are calculated with the piecewise finite-element-function ϕ_l and we get

$$\nabla c_{jk}^{e,n+1} = \sum_{l \in \Lambda^e} c_l^{n+1} \nabla \phi_l(\mathbf{x}_{jk}^e)\ . \tag{37}$$

Using the difference-notation for the neighbor-points j and l, confer [12], leads to the following discretization form.

$$\begin{aligned} &V_j R(c_j^{n+1}) - V_j R(c_j^n) = \\ &= \tau^n \sum_{e \in \Lambda_j} \sum_{l \in \Lambda^e \setminus \{j\}} \Big(\sum_{k \in \Lambda_j^e} |\Gamma_{jk}^e| \mathbf{n}_{jk}^e \cdot D_{jk}^e \nabla \phi_l(\mathbf{x}_{jk}^e) \Big) (c_j^{n+1} - c_l^{n+1})\ , \end{aligned} \tag{38}$$

where $j = 1, \ldots, m$.

In the next section we describe the analytical solutions for the new discretization-methods of the convection-reaction-equation based on finite volume methods.

5 Analytical solutions

For the next section we transformed our equations to the following system of one-dimensional convection-reaction-equations without diffusion. The equations are given as

$$\partial_t c_i + v_i \partial_x c_i = -\lambda_i c_i + \lambda_{i-1} c_{i-1}\ , \tag{39}$$

for $i = 1, \ldots, m$. The unknown m is the number of components. The unknown functions $c_i = c_i(x,t)$ denote the contaminant concentrations. They are transported with piecewise constant (and in general different) velocities v_i. They decay with constant reaction rates λ_i. The space-time domain is given by $(0, \infty) \times (0, T)$.

We assume simple (irreversible) form of decay chain, e.g. $\lambda_0 = 0$, and for each contaminant only a single source term $\lambda_{i-1} c_{i-1}$ is given. For simplicity we assume that $v_i > 0$ for $i = 1, \ldots, m$.
We describe the analytical solutions with piecewise linear initial conditions. But also all other piecewise polynomial functions could be derived, confer [14].

For boundary conditions we take zero concentrations at inflow boundary $x = 0$ and the initial conditions are defined for $x \in (0, 1)$ with

$$\begin{aligned} c_1(x,0) &= \begin{cases} ax + b\,, & x \in (0,1) \\ 0 & \text{otherwise} \end{cases}\,, \\ c_i(x,0) &= 0\,, \quad i = 2, \ldots, m\,, \end{aligned} \tag{40}$$

where $a, b \in I\!R^+$ are constants.

The Laplace-Transformation is used for the transformation of the partial differential equation into the ordinary differential equation, described in [16]. The ordinary differential equations are solved and the solutions are described in [5]. We re-transformed the solution in the original space of the partial differential equations. We could then use the solution for the one-dimensional convection-reaction-equation, confer [14].

The solutions are given as

$$c_1(x,t) = \exp(-\lambda_1 t) \begin{cases} 0 & , \; 0 \le x < v_1 t \\ a(x - v_1 t) + b & , \; v_1 t \le x < v_1 t + 1 \\ 0 & , \; v_1 t + 1 \le x \end{cases}\,, \tag{41}$$

$$c_i(x,t) = \Lambda_i \left(\sum_{j=1}^{i} \exp(-\lambda_j t) \Lambda_{j,i} \sum_{\substack{k=1 \\ k \neq j}}^{i} \Lambda_{jk,i} A_{jk} \right)\,, \tag{42}$$

$$A_{jk} = \begin{cases} 0 & , \; 0 \le x < v_j t \\ a(x - v_j t) & \\ +(b - \frac{a}{\lambda_{jk}})(1 - \exp(-\lambda_{jk}(x - v_j t))) & , \; v_j t \le x < v_j t + 1 \\ (b - \frac{a}{\lambda_{jk}} + a) \exp(-\lambda_{jk}(x - v_j t - 1)) & \\ -(b - \frac{a}{\lambda_{jk}}) \exp(-\lambda_{jk}(x - v_j t)) & , \; v_j t + 1 \le x \end{cases} \tag{43}$$

where the general solutions have the following definition-array
$v_i \neq v_j$, $\lambda_i \neq \lambda_j$, $\lambda_{ij} \neq \lambda_{ik}$ and $v_i \neq v_j \;\wedge\; \lambda_i \neq \lambda_j$,
$\forall\, i, j, k = 1, \ldots, M$, if $i \neq j \wedge i \neq k \wedge j \neq k$.

The further abbreviation for λ_{jk} and Λ_i are

$$\lambda_{kj} = \lambda_{jk} := \frac{\lambda_j - \lambda_k}{v_j - v_k}\,, \;\; \Lambda_i := \prod_{j=1}^{i-1} \lambda_j\,, \tag{44}$$

and the factors $\Lambda_{j,i}$ and $\Lambda_{jk,i}$ are

$$\Lambda_{j,i} = \left(\prod_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_k - \lambda_j} \right) , \Lambda_{jk,i} = \left(\prod_{\substack{l=1 \\ l \neq j \\ l \neq k}}^{i} \frac{\lambda_{jl}}{\lambda_{jl} - \lambda_{jk}} \right) . \tag{45}$$

The solutions are used in the discretization methods for the embedded analytical mass. To complete the study for the analytical solutions, we introduce the special solutions for the equal reaction-parameter $\lambda_l = \lambda_{a(l)}$.

5.1 Mass reconstruction and Analytical solution of the Mass

For the embedding of the analytical mass in the discretization method, we need the mass transfer of the norm-interval $(0, 1)$. We use the fact that reconstruction is given by the total mass as

$$m_{i,sum}(t) = m_{i,rest}(t) + m_{i,out}(t) \tag{46}$$

The integrals are computed over the normed cell $(0, 1)$. We integrate first the mass that retains in the cell i and then we calculate the total mass. The difference between the total mass and the residual mass is the out-flowing mass which is used for the discretization.

We have derived the residual mass, confer [14], and it is denoted as

$$\begin{aligned} m_{i,rest}(t) &= \prod_{j=1}^{i-1} \lambda_j \sum_{j=1}^{i} \Big(\prod_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_k - \lambda_j} \Big) \\ & \exp(-\lambda_j t) \left(a \frac{(1 - v_j t)^2}{2} + b(1 - v_j t - \sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}}) \right. \\ & \left. -a(1 - v_j t)(\sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}}) + a\Big(\sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}} (\sum_{\substack{l \geq k \\ l \neq j}}^{i} \frac{1}{\lambda_{jl}}) \Big) \right) , \end{aligned} \tag{47}$$

where the parameters λ_{jk} are given in the equation (44) .

The total mass is calculated by the solution of the ordinary equation and the mass of the initial condition. The solution of the total mass is derived as

$$m_{i,sum}(t) = \prod_{j=1}^{i-1} \lambda_j \Big(\sum_{j=1}^{i} \Big(\prod_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_k - \lambda_j} \Big) \exp(-\lambda_j t) \Big) (\frac{a}{2} + b) .$$

The out-flowing mass is defined for further calculations

$$m_{i,out}(\tau^n) = m_{i,sum}(\tau^n) - m_{i,rest}(\tau^n) \ , \tag{48}$$
$$m_{i,out}(\tau^n) = m_{i,out}(a, b, \tau^n, v_1, \ldots, v_i, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i) \ , \tag{49}$$
$$m_{i,sum}(\tau^n) = f_i^n \ (a\frac{1}{2} + b) \ , \tag{50}$$
$$f_i^n(\tau^n) = f(\tau^n, v_1, \ldots, v_i, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i) \ , \tag{51}$$

whereby τ^n is the time-step, $v_1, \ldots, v_i$ are the velocity-, $R_1, \ldots, R_i$ are the retardation- , $\lambda_1, \ldots, \lambda_i$ the reaction-parameters and a, b are the parameters for the linear impulse for the initial conditions.

In the next section we describe the used solvers for the implicit time-discretized equations. We introduce the solver based on multi-grid methods.

6 Solvers

For solving the implicit discretized diffusion-dispersion equation or the diffusion-dominant convection-diffusion equation, we use iterative methods. The discretization results in the linear system of equations $Ax = b$. Because of the local discretization method and the knowledge of the stabile solvers for this kind of equations, we use the Multi-grid-solvers to solve our equation. These solver methods are used for this type of parabolic equations, confer [18]. We could use the standard convergence-results of these methods.

We will briefly introduce the methods and for an intensive study we refer to the literature [29], [28].

We have the following linear equation-system

$$Ax = b \ , \ A \in I\!R^{I \times I} \ , \ b \in I\!R^I \ , \tag{52}$$

whereby A is regular, x is the unknown and b is the right hand side.

The iteration-method is given as :

$$x^{m+1} = Mx^m + Nb \ , \quad m \in I\!N \ , \tag{53}$$

whereby b is the right-hand side. and we get a consistent iteration-method for

$$M = \mathbb{1} - NA \ . \tag{54}$$

whereby $\mathbb{1}$ is the identity matrix. The matrix M is denoted as iteration-matrix.

We could modify equation (53) for the second normal-form given as

$$x^{m+1} = x^m - N(Ax^m - b) \ . \tag{55}$$

The iteration-method is applied for the multi-grid method [18].
We introduce the multi-grid methods

$$M_0^{MG} := 0 \,, \tag{56}$$

$$M_1^{MG} := M_1^{ZG} \,, \tag{57}$$

$$M_l^{MG} := M_l^{ZG} + \; S_l^{\nu_2} \; p \; (M_{l-1}^{MG})^{\gamma} \; A_{l-1}^{-1} \; r \; A_l \; S_l^{\nu_1} \,, \tag{58}$$

where S_l is the smoother, p is the prolongation, r is the restriction, ν_1 are the pre-smoothing steps and ν_2 the post-smoothing-steps. The coarse-grid correction M_l^{MGG} is defined as

$$M_l^{MGG} \; := \; \mathbb{1} - p \; (I - (M_{l-1}^{MG})^{\gamma}) \; A_{l-1}^{-1} \; r \; A_l \,. \tag{59}$$

We use these iteration-methods to solve our equations on a grid-hierarchy, confer [14].

In the next section we introduce our used R^3T-software-tools.

7 Software-tools R^3T

The methods introduced in the last sections are programmed in our flexible software-tool R^3T. The software package R^3T is developed for solving 2d and 3d transport- and reaction-equations for multiple species in flowing groundwater based on a porous media. We developed the solutions of convection-dominant equations and improved the discretizations to use coarser grids and therefore larger time-steps. The package includes the error-estimators, solvers and discretization methods. We have developed nonlinear solvers for our nonlinear reaction-equations. For the parameter of the equation and the velocity-field we use input-files to set the different values. These dates are read in run-time and for a new run we could change the values for a new configuration. The solutions of the equations are written in output-files and could be used for different post-processors. We have visualized our results with the visualization-program Grape [17]. For the testing we use different waste-case scenarios for different initial conditions, see section 8. The methods are separately tested in various one- and two-dimensional test-cases with underlying analytical solutions.

The tool *R3T* is based on the software-tool *ug*, confer [2], which is based on unstructured grid. The methods for these unstructured grids are programmed in different libraries and are modular programmed. Based on the grid-hierarchy, the solvers, e.g. multi-grid solvers, discretization-methods with respect of adaptive methods are programmed. The idea behind is a flexible tool with common libraries of solvers, discretization-methods, error-estimators and a flexible application-level for applications in physical- and chemical-models.

The applications are presented in the next section with benchmark and waste-case scenarios.

8 Numerical experiments

In the first part we introduce a numerical example with analytical solutions to verify our underlying numerical method. In the second part we present a numerical example for a waste-disposal in 2d in a complex domain.

8.1 Waste-Case Scenarios

We calculate scenarios of waste-cases which help to get new conclusions about the waste-disposals in salt-domes.

We have a model based on an overlying-rock over a salt-dome. We suppose a waste-case, so that a permanent source of radioactive contaminant groundwater flows from the bottom of the overlying rock, where the waste-disposal is suited. We suppose that the contaminants are flown with the groundwater, which is flown through the overlying rock. Based on our model we should calculate the transport and the reaction of these contaminants coupled with decay-chains. The simulation time should be 10000$[a]$ (where $[a]$ is shortened as years) and we should calculate the concentration that is flown till the top of the overlying rock. With these data one could conclude if the waste-disposal is save enough.

Two cases are next presented with the realistic data. The first case is a benchmark-example. The second case is a scenario with a possible domain and realistic model parameters, confer [7] and [8].

8.2 First example for a waste scenario

We introduce a benchmark-problem for a possible example for a waste-scenario. For this scenario an analytical solution is derived and we could compare the different solutions. The example is calculated with realistic parameters.

A realistic potential waste scenario is simulated for a waste disposal for radioactive contaminants.

For simplicity we reduce the model-domain to an one-dimensional model-domain. For this domain we could apply our analytical methods. We simulate the convection-reaction-equation for long time-scales.

The realistic parameters are used from a long-time-analysis for a waste-disposal. We could use this experiment to simulate a waste-disposal for a simple domain, but with respect to the domain-scales of our original domain. For this example the analytical solutions exist and therefore we could compare the numerical solutions. The retardation- and exchange-processes could be simulated with this example.

The calculations are used as a pre-step before the more complex models in 2d and 3d, for which no analytical solutions are known for arbitrary domains and parameters.

The following example is a decay-chain for the Neptunium-row and presents the strong variation in the retardation and decay-factors with respect of large scales, where in the following $[s]$ is shortened as seconds).

The decay-chain is given as
Am-241 $\rightarrow$ Np-237 $\rightarrow$ U-233 $\rightarrow$ Th-229 .

The retardation-factors are
$R_{Am} = 200.2$, $R_{Np} = 2.2$, $R_U = 1.6$, $R_{Th} = 2000.2$.

The porosity is $\phi = 0.5$.

The decay-rates are
$T_{1/2,Am} = 1.3639\ 10^{10}\ [s]$, $T_{1/2,Np} = 6.7659\ 10^{13}\ [s]$,
$T_{1/2,U} = 15.0239\ 10^{12}\ [s]$, $T_{1/2,Th} = 2.4867\ 10^{11}\ [s]$.

For our simulations we consider a time-period of 6340 $[a]$. The time-step-width is restricted with a time-step control, for which we use the Courant-number 0.5, confer [14]. The domain of our model is 8000 $[m] \times 1000\ [m]$.

The initial-conditions are given as a triangle-impulse with the length 500 $[m]$. The impulse is spread out in the y-direction, we have therefore an one-dimensional test-example. The initial concentration is 1.0.
The boundary-conditions are trivial inflow- and outflow-conditions, where $\mathbf{n} \cdot \mathbf{v}\ c_i = 0$. There will be no source-terms, e.g. $\tilde{Q}_i = 0.0$ for $i = 1, \ldots, 4$.

The velocity is one-dimensional in x-direction and constant in the domain with $\mathbf{v} = (2 \cdot 10^{-8}, 0)^T\ [m/s]$.

We compute the error-norms and convergence-orders for the numerical results for the different grid-levels.

We use the operator-splitting method as standard-method and discretize with finite volume-methods the convection-equation and with analytical solution the reaction equation. We use our new discretization method with embedded analytical solutions for our modified method and could skip the splitting-error.
The standard- and modified methods are compared in the following subsections.

Standard-Method

In the following computations we use the standard-methods for our calculations. The errors are computed with the L_1-norm. The absolute error is calculated between the numerical and analytical solutions.

The large scale-differences reached over multi-decimal scales are transferred to the absolute errors of the computations. In Table 1 are presented the results for the absolute errors.

The numerical convergence-orders are calculated with the absolute errors and presented in Table 2.

l	$E^1_{L_1}$	$E^2_{L_1}$	$E^3_{L_1}$	$E^4_{L_1}$
4	$4.13\ 10^{-1}$	$1.96\ 10^{6}$	$2.71\ 10^{3}$	$3.14\ 10^{-4}$
5	$1.59\ 10^{-1}$	$8.62\ 10^{5}$	$1.31\ 10^{3}$	$9.55\ 10^{-5}$
6	$5.66\ 10^{-2}$	$4.28\ 10^{5}$	$6.52\ 10^{2}$	$4.20\ 10^{-5}$
7	$2.1\ 10^{-2}$	$2.15\ 10^{5}$	$3.26\ 10^{2}$	$1.66\ 10^{-5}$

Table 1: The absolute L_1-error for the standard-method for the one-dimensional model-problem and realistic parameters.

l	$\rho^1_{L_1}$	$\rho^2_{L_1}$	$\rho^3_{L_1}$	$\rho^4_{L_1}$
4	-	-	-	-
5	1.58	1.18	1.04	1.7
6	1.44	1.01	1.006	1.18
7	1.43	0.99	1.0	1.2

Table 2: The convergence-order for the L_1-errors for the standard-method for the one-dimensional model-problem and the realistic parameters.

Therefore the smooth initial-impulses for the first components are of higher convergence-order. The next components calculated with the standard-method are of convergence-order 1. The standard-method has for the higher components low order results. We improve the results with our new modified method.

Modified method

The numerical calculations with the modified method are compared with the analytical solutions in the L_1-norm. In Table 3 we give the L_1-errors.

l	$E^1_{L_1}$	$E^2_{L_1}$	$E^3_{L_1}$	$E^4_{L_1}$
4	$4.13\ 10^{-1}$	$1.19\ 10^{6}$	$3.188\ 10^{2}$	$4.355\ 10^{-4}$
5	$1.54\ 10^{-1}$	$2.46\ 10^{5}$	$5.33\ 10^{1}$	$5.66\ 10^{-5}$
6	$5.66\ 10^{-2}$	$8.92\ 10^{4}$	$1.13\ 10^{1}$	$1.02\ 10^{-5}$
7	$2.10\ 10^{-2}$	$2.35\ 10^{4}$	$2.89\ 10^{0}$	$2.89\ 10^{-6}$

Table 3: The absolute L_1-error for the modified method with the one-dimensional model-problem and the realistic parameters.

The numerical convergence-orders for the modified method is given in Table 4.

The modified method satisfied our improved methods with the higher order convergence-results which are described in the theory of the large scale

l	$\rho^1_{L_1}$	$\rho^2_{L_1}$	$\rho^3_{L_1}$	$\rho^4_{L_1}$
4	-	-	-	-
5	1.58	2.27	2.58	2.94
6	1.44	1.58	2.23	2.47
7	1.43	1.93	1.967	1.72

Table 4: The convergence-order with the L_1-errors for the modified method with the one-dimensional model-problem and the realistic parameters.

problems.

The results are displayed graphically. The initial-condition for the for the first component are presented in Figure 1.

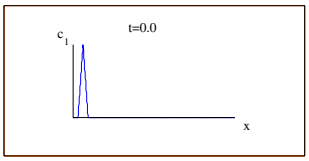

Figure 1: Initial-condition of the first component in the time $t = 0$ $[a]$.

In the next presentations in Figure 2 we display the propagation of the components till the end-time-point 6340 $[a]$.

The first component is most retarded and therefore less transported. The second and third components are less retarded and more transported. The fourth component is at most retarded and very less transported. Because of the coupling through the decay with the predecessor-components the impulse is spread out till the predecessor concentration.

In the next section we describe a two dimensional waste-case with different sources.

8.3 Second waste-case : Two Dimensional Model with different sources

We have a model-domain in the size of $6000[m] \times 150[m]$ with 4 different layers with different permeabilities, confer [7]. The domain is spooled with groundwater from the right boundary to the left boundary. The groundwater is flowing faster through the permeable layer than through the impermeable layers. Therefore the groundwater flows from the right boundary to the half middle of the domain. It is flowing through the permeable layer down to the bottom of the domain and spools up in the left domain to the top. The

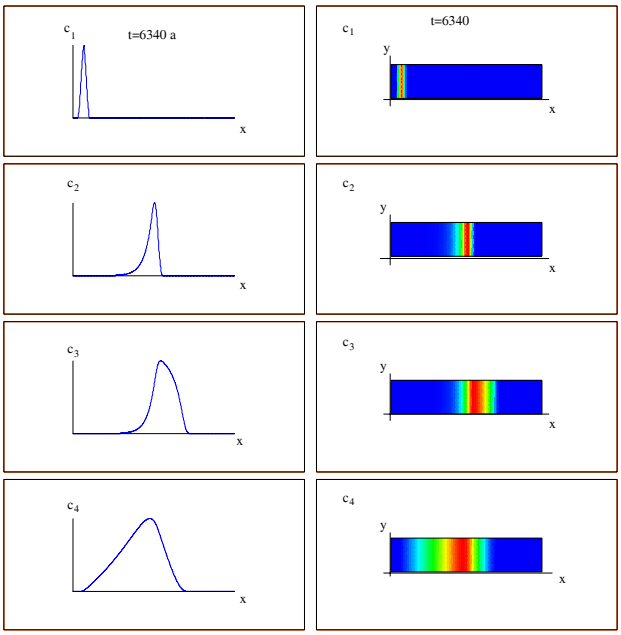

Figure 2: The propagation of the contaminants after 6340 $[a]$ with an one-dimensional cut and a color plot.

groundwater flows in the left top part to the outflow at the left boundary. The flow-field with the velocity is calculated with the program-package $\mathbf{d^3f}$ and presented in Figure 3.

In the middle-bottom of the domain the contaminants are flown in as a permanent source. With the stationary velocity-field the contaminants are computed with the software-package R^3T. The flow-field transports the radioactive contaminants till the top of the domain. The decay-chain is presented with 26 components as follows

$$
\begin{aligned}
&Pu-244 \rightarrow Pu-240 \rightarrow U-236 \rightarrow Th-232 \rightarrow Ra-228\\
&Cm-244 \rightarrow Pu-240\\
&U-232\\
&Pu-241 \rightarrow Am-241 \rightarrow Np-237 \rightarrow U-233 \rightarrow Th-229\\
&Cm-246 \rightarrow Pu-242 \rightarrow U-238 \rightarrow U-234 \rightarrow Th-230 \rightarrow\\
&Ra-226 \rightarrow Pb-210\\
&Am-242 \rightarrow Pu-238 \rightarrow U-234\\
&Am-243 \rightarrow Pu-239 \rightarrow U-235 \rightarrow Pa-231 \rightarrow Ac-227\ .
\end{aligned}
$$

We concentrate on the important decay-chain :
$Am-243 \rightarrow Pu-239 \rightarrow U-235$.

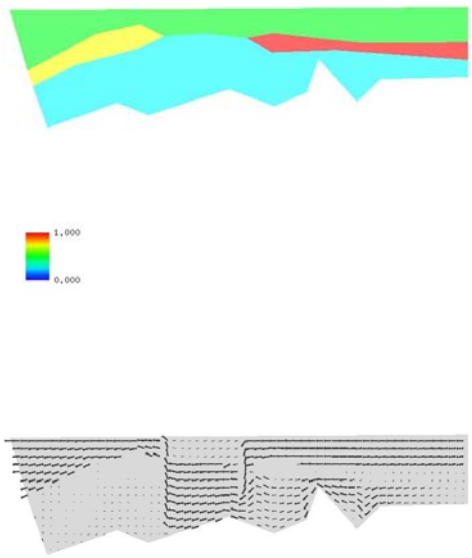

Figure 3: Domain with different layers and Flow-field for a two-dimensional calculation.

We present the important concentration in this decay-chain. In the top figure 4 the contaminant Uranium-isotope U-236 after 100[a] is presented. This isotope is less retarded and has a very long half-life period. Therefore the contaminant is flown as furthest and decays less. This effect is presented in bottom figure 5. The diffusion-process has spread out the contaminant in the whole left part of the domain. Also the impermeable layer is contaminated. After the time-period of 10000[a] the contaminant is flown till the top of the domain.

The calculations are done on uniform grids. The convergence of these grids are confirmed with adaptive grid-calculations. The calculation confirmed the results of finer and smaller time-steps, confer table 5. The beginning of the calculations is done with explicit methods till the character of the equations is more diffusive-dominant. Then we change to the implicit methods and could use larger time-steps. With this procedure we could fulfill the forced calculation time of maximal one day.

The calculations are done with Athlon-processors on a 64 Bit-architecture with 1.4 GHz.

Finally we conclude in our paper with the next section.

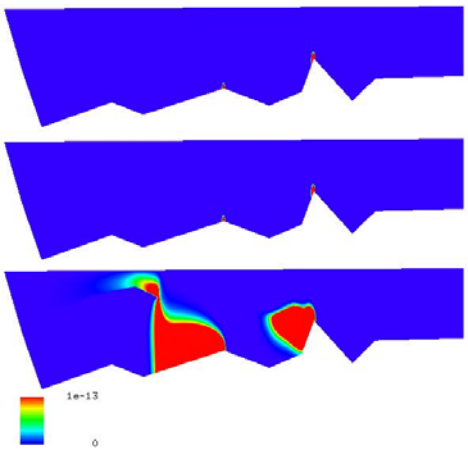

Figure 4: Concentration of U-236 at the time-point $t = 300[a]$ and different concentrations.

Processors	Refinement	Number of Elements	Number of Time-steps	Time for one time-step	Total Time
64	uniform	2437120	5000	26.7 sec.	37.5 h.
256	uniform	9748480	5000	28.5 sec.	40.5 h.

Table 5: Computing of the two-dimensional case and different wells.

9 Conclusions and Discussions

We present a discretization and solver methods for solving a complex system of convection-diffusion-dispersion-reaction equations. Based on the decoupling idea we discretized our simpler equations with higher order methods. With a new technique of embedded analytical solution we improve the standard discretization methods. The analytical solutions for the simpler equations and their application in our methods are described. We presented our solvers and the fundamental program-tool. The examples for the waste-disposals are presented in a benchmark-scenario and a realistic scenario.

We confirmed that a complex model can be simulated with the help of discretization and solver methods.

In the future we focus on the development of improved discretization methods with respect to their parallel applications and on the idea of constructing splitting-methods of higher order for decoupling in simpler nonlinear convection-diffusion-reaction-equations.

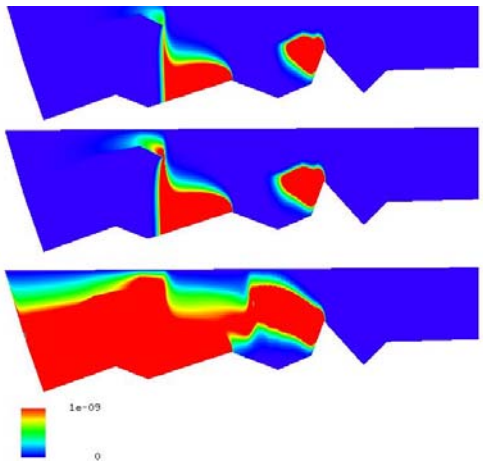

Figure 5: Concentration of U-236 at the time-point $t = 1000[a]$ and different concentrations.

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